



Computational Design of Materials: From Planetary Entry to Electric Aircraft and Beyond

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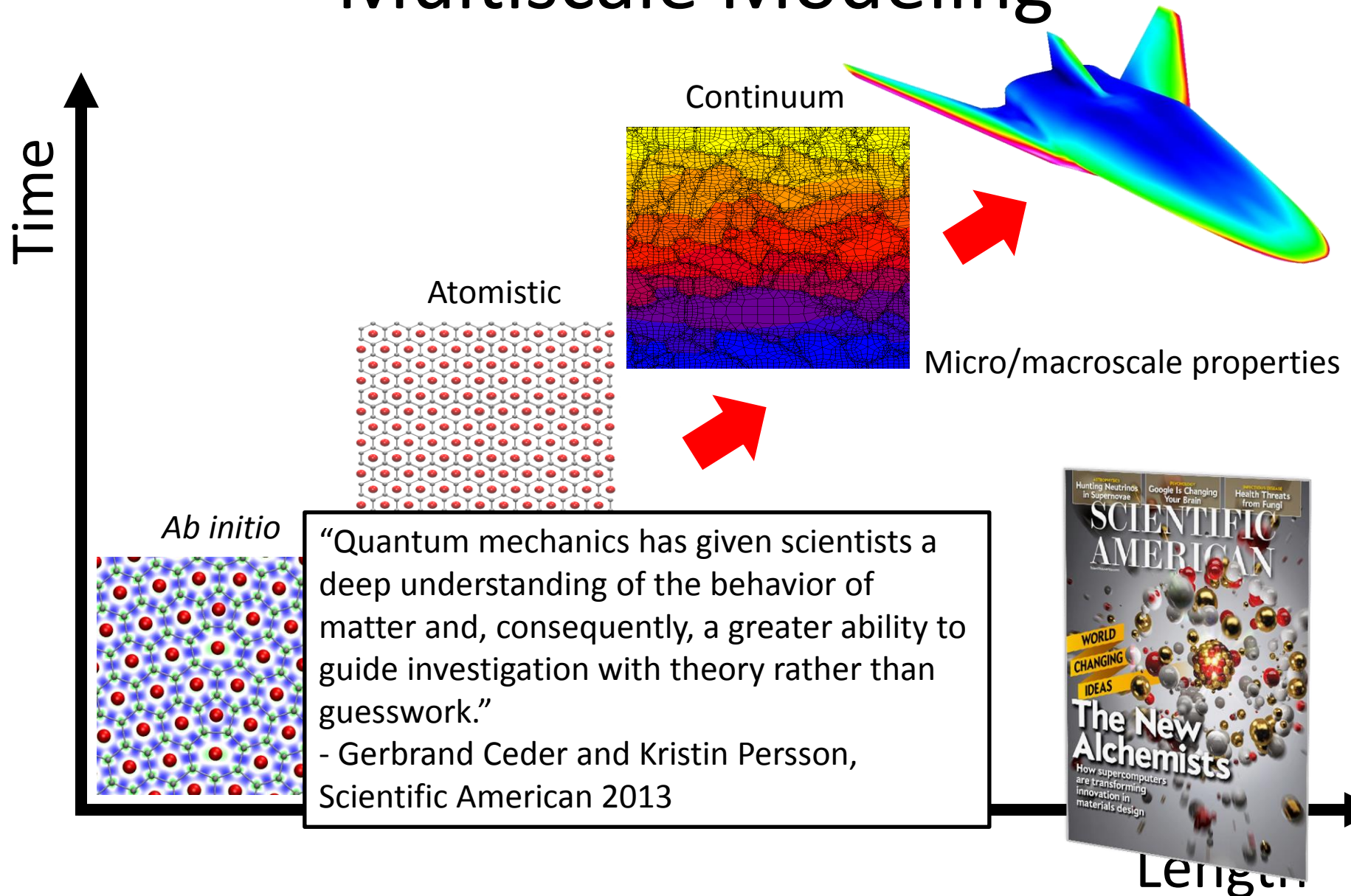
Computational Materials Design

- Materials design is a slow, expensive process
 - Estimated 15-20 years
- Computational materials science can help
 - Pinpoint important design factors
 - Screen new materials
 - Suggest promising candidates

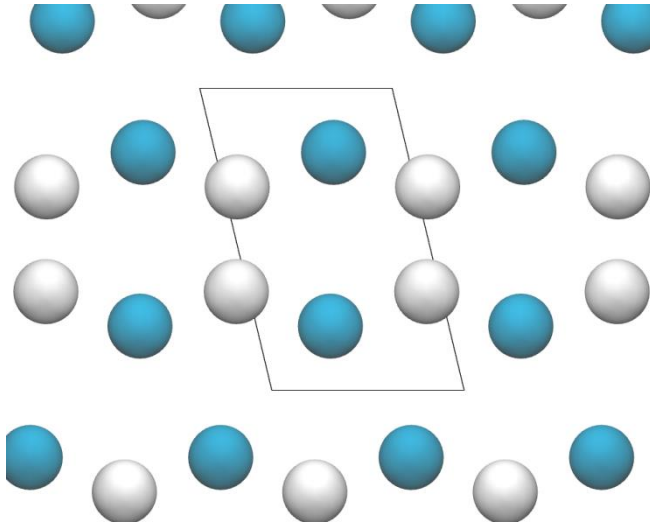
“The ultimate goal is to generate computational tools that enable real-world materials development, that optimize or minimize traditional experimental testing”
- The White House’s White Paper on the Materials Genome Initiative 2011



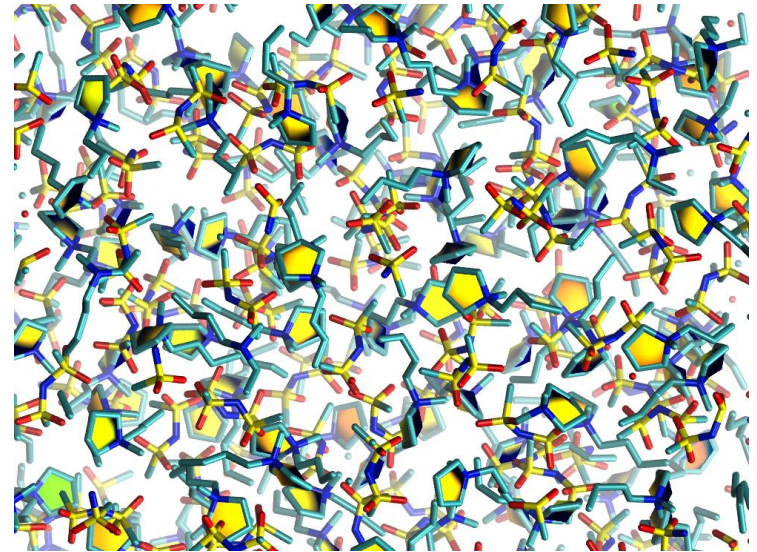
Multiscale Modeling



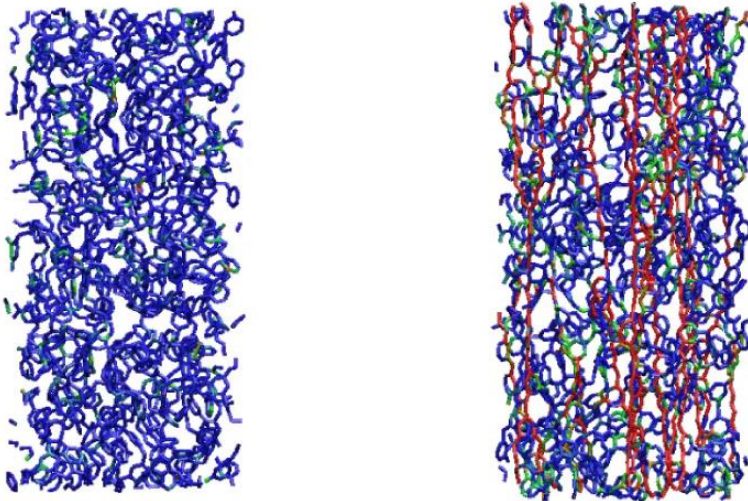
Shape Memory Alloys



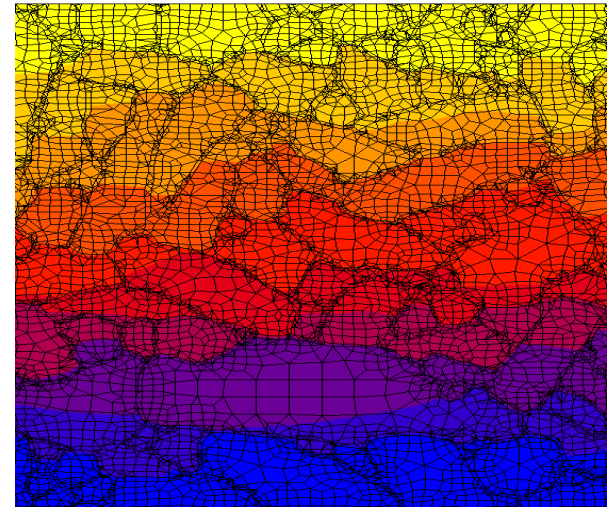
Advanced Electrolytes for Batteries



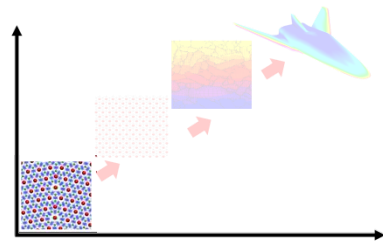
Ablative Materials for Reentry



Ultra High Temperature Ceramics



Shape memory alloys (SMAs)



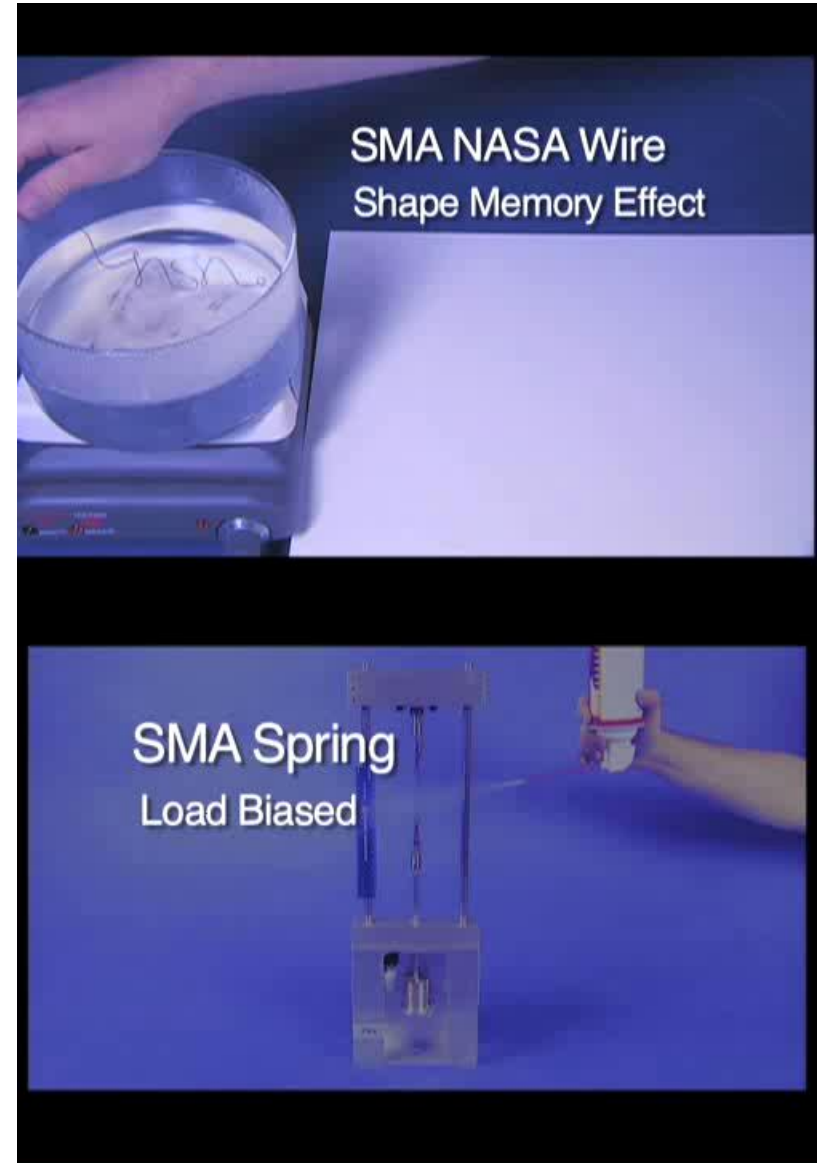
What is a SMA?

Deformations at low temperature can be reversed at high temperature.

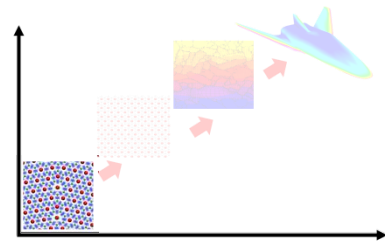
SMAs could be a lightweight actuator for airplanes

- No motor needed
- Only need heat

Problem: Need higher transition temperatures for aeronautic applications



Shape memory alloys (SMAs)

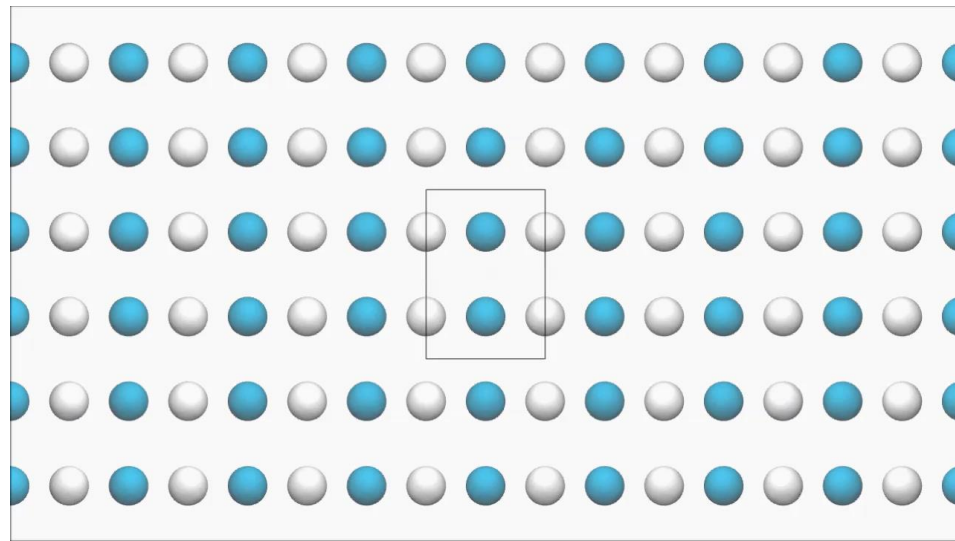
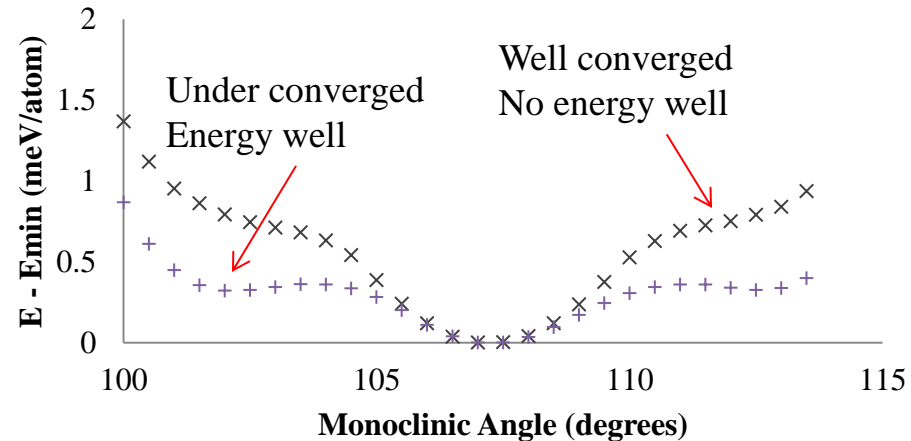


Project overview: Predict phase transition temperature from first principles.

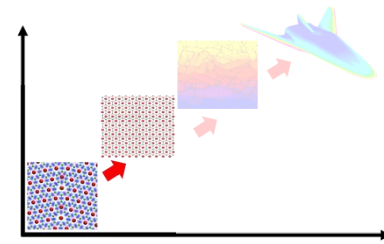
Role of Supercomputing: Extensively probe computational parameters and convergence criterion. Run long, heavy dynamics calculations.

Milestone: Determine energetic and mechanical stability of phases with *ab initio* calculations. We show that previously reported intermediate phases are likely artifacts of poorly converged calculations.

NiTi energy landscape



Batteries for electric aircraft



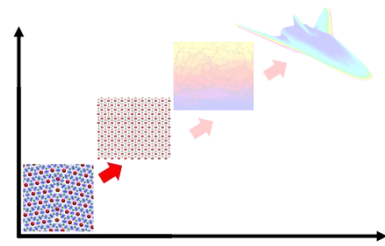
Why batteries for planes?: Aircraft release greenhouse gasses high in the atmosphere, where they are most damaging. Batteries can be an alternative to fossil fuels in planes.

Problem: Need higher energy density and better safety.

- Lithium metal electrodes can increase energy density, but can fail.
- Advanced ionic electrolytes could enable lithium electrodes, but need to be characterized.



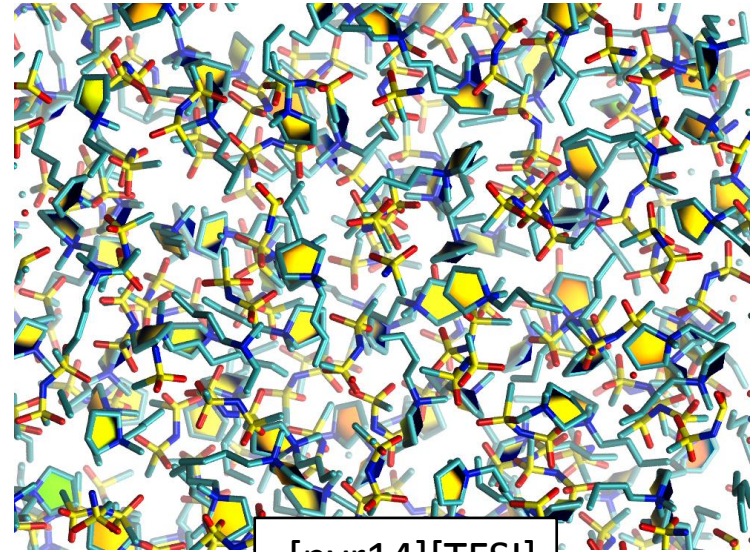
Batteries for electric aircraft



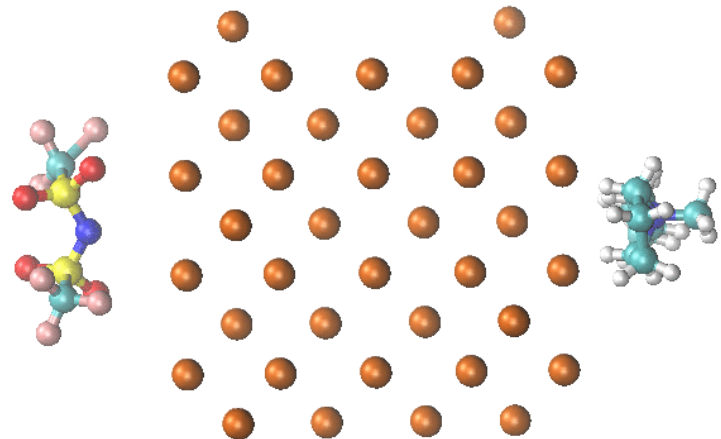
Project overview: Study ionic liquid electrolytes that enable lithium metal anodes

Role of Supercomputing: In order to get realistic thermal behavior at room temperature, we needed to simulate the electrolyte for 200 nanoseconds (an eternity in atomistic calculations!)

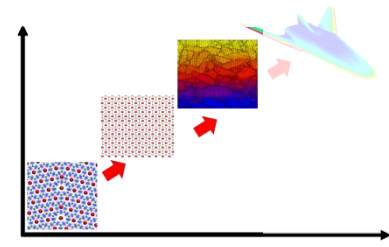
Milestone: Characterize differences between known electrolytes to determine important design factors



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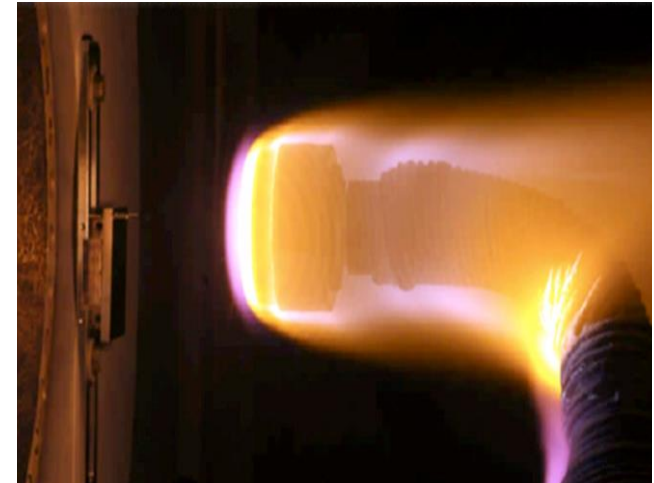
Ablative Materials for Reentry



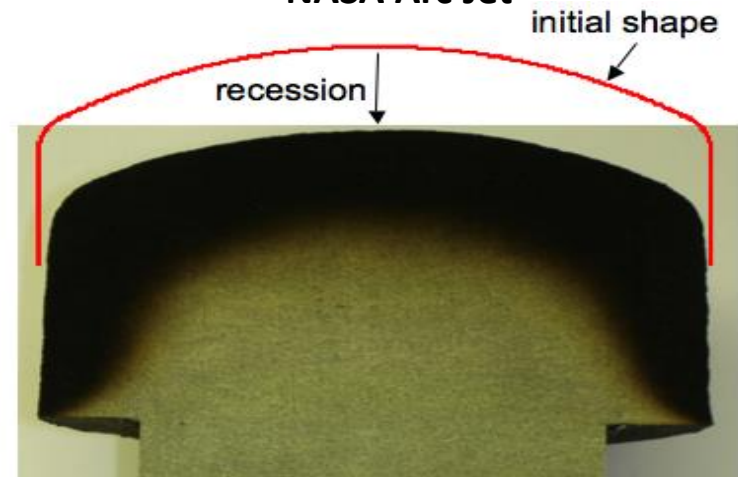
What are ablative materials?: Ablative materials are used to slow the decent of spacecraft through atmospheres— Earth, Mars, and beyond.

Future space missions will require more robust thermal protection.

Problem: It is not known how the geometry of individual polymer chains affects the macroscale properties.

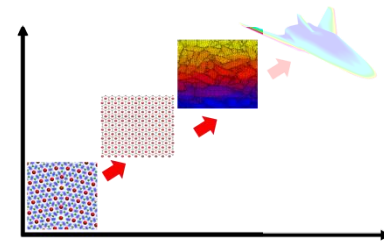


NASA Arc Jet



Arc jet sample with charred surface

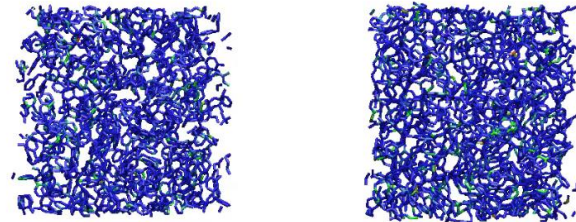
Ablative Materials for Reentry



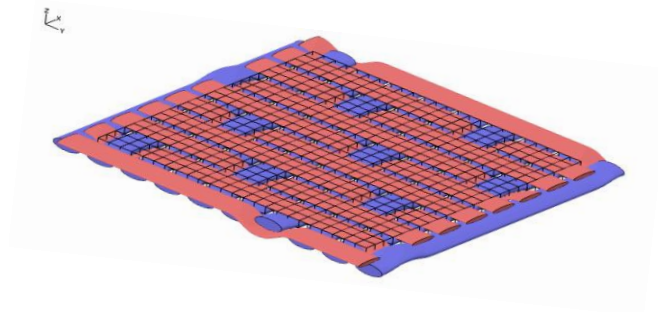
Project overview: Characterize chemical, thermal, and mechanical properties of ablative materials

Role of Supercomputing:

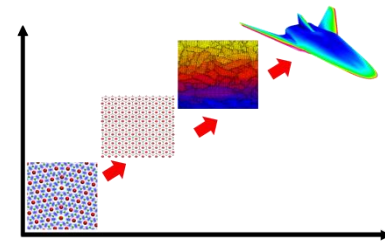
Thermal conductivity requires long simulation times (100 nanoseconds). Properties calculated across a range of cross-linking.



Milestone: Calculated thermal expansion, thermal conduction, and elastic moduli at atomic scale for input at macro-scale.



Ultra High Temperature Ceramics



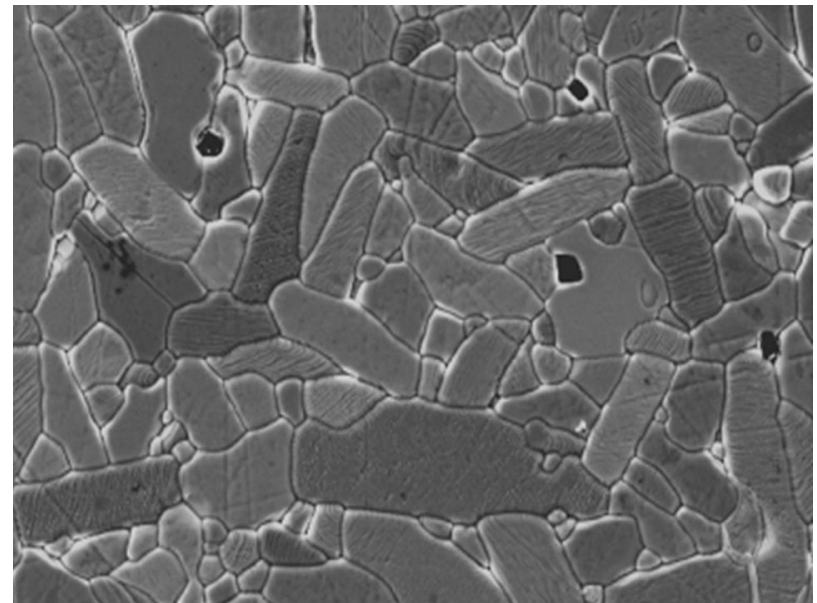
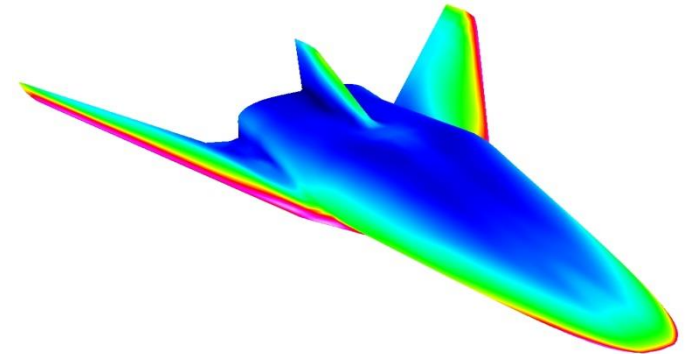
What are UHTCs? These materials can endure in hot, extreme environments, like the leading edge of aircraft wings.

Sharp leading edges of aircraft improve performance and safety.

However, they also increase temperature requirements:

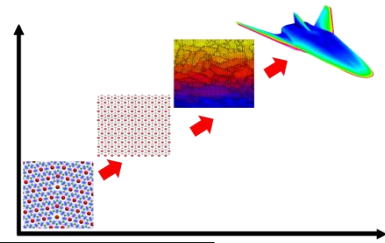
- Shuttle RCC leading edge: $T \sim 1650\text{ }^{\circ}\text{C}$
- Sharp leading edges: $T > 2000\text{ }^{\circ}\text{C}$

Problem: Need to characterize thermal performance of these materials.



Grain boundaries are a limiting factor for thermal conduction

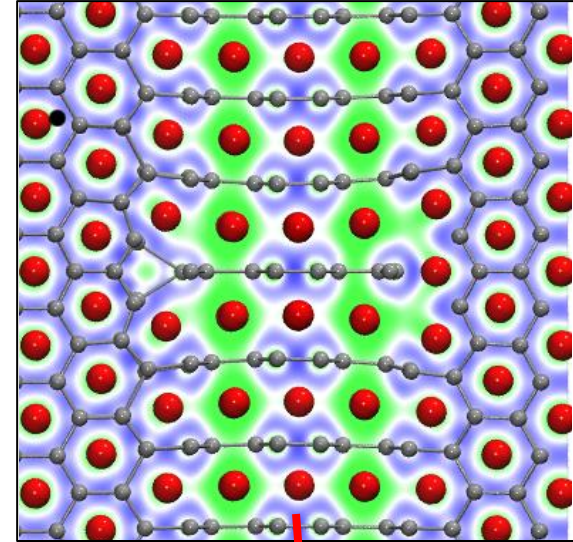
Ultra High Temperature Ceramics



Project overview: Characterize thermal properties zirconium diboride perfect crystals (bulk) and defects (grain boundaries).

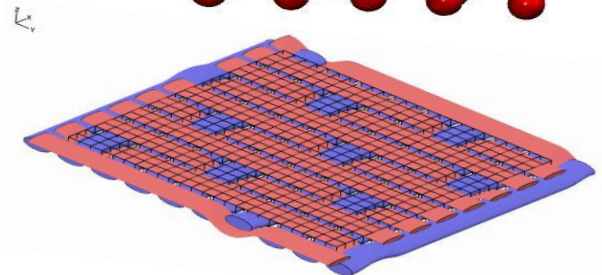
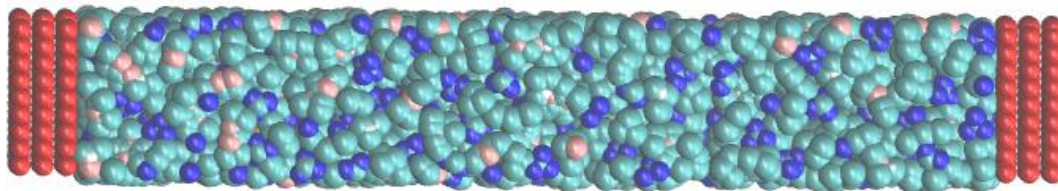
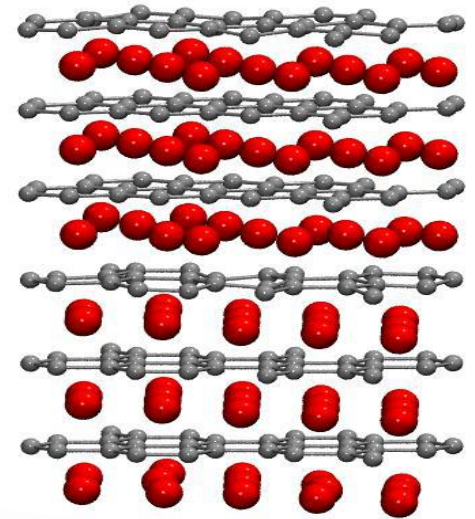
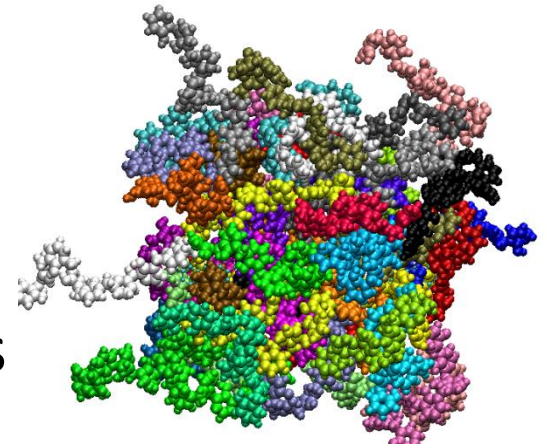
Role of Supercomputing: Grain boundary calculations are computationally intensive because they necessarily contain many atoms and there are many types to calculate.

Milestone: Calculate thermal conductivity of grain boundaries and bulk to pass onto finite element method calculations



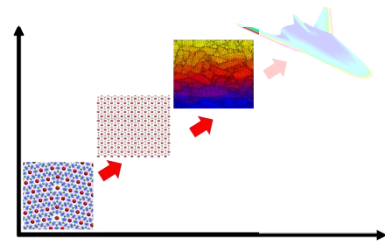
Summary

- Important physics and chemistry occurring at varied length/time scales
- Multiscale modeling captures these different levels, feeding one into the next
- Can model a material starting from quantum mechanics (parameter free!)
- Broadly applicable to many materials
- Explanatory value/Guides experiments

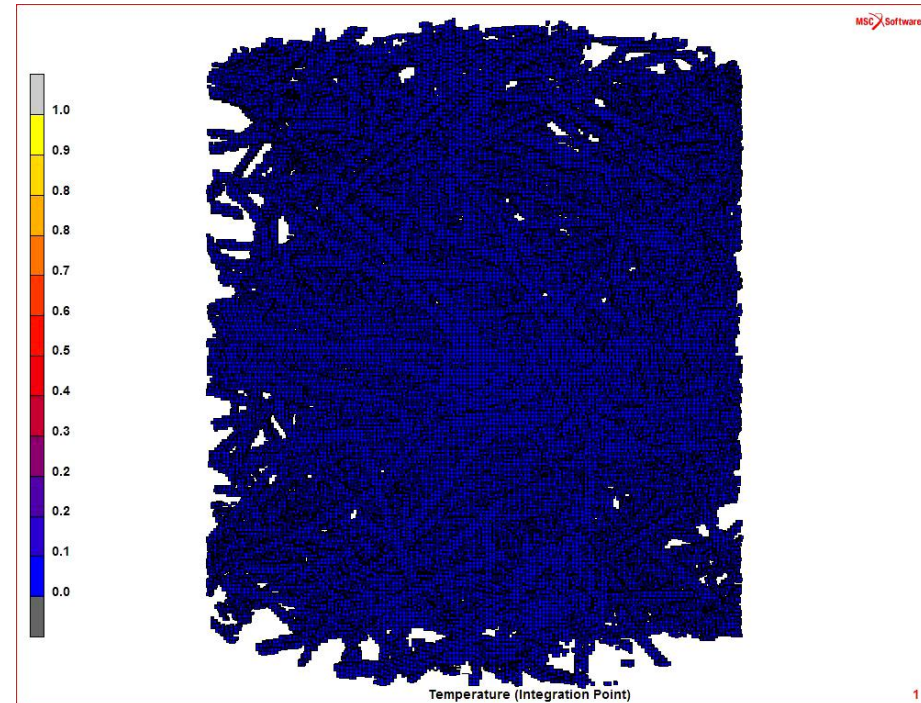
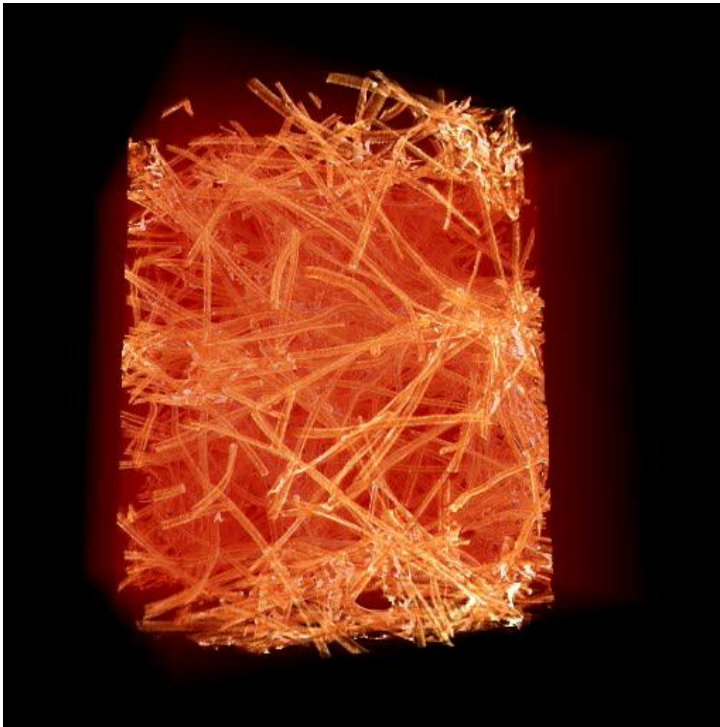


Extras

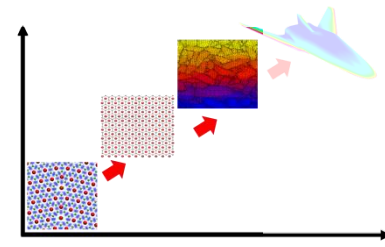
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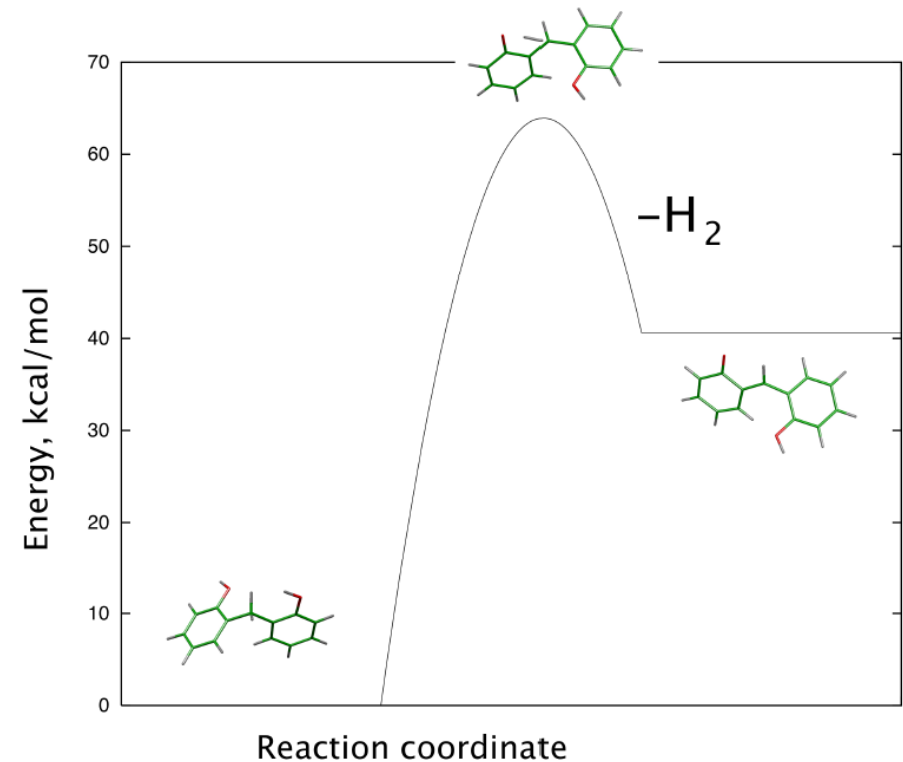
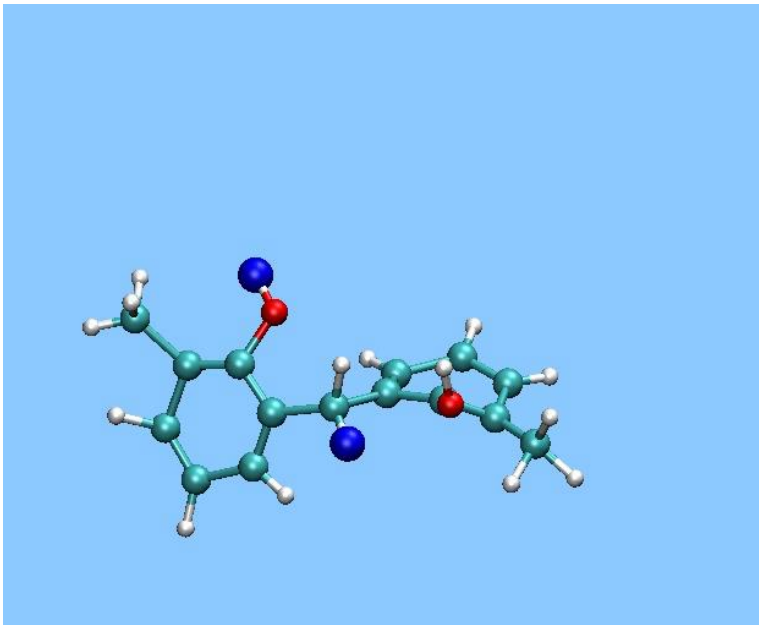
Use CT scan of ablative fibers to realistically model 3D microstructure. Use thermal properties from molecular dynamics calculations to model conduction of heat across a sample.



Ablative Materials for Reentry



Pyrolysis of PICA



Interactive animation of NiTi

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